IR SPECTROSCOPIC AND THEORETICAL STUDY OF NEW PHOTOCHROMIC SYSTEMS BASED ON CYMANTRENE DERIVATIVES.

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New photochromic systems based on cymantrene derivatives (η^5-C_5H_4R)Mn(CO)$_3$ containing mono- and bifunctional n-donor and π-donor substituents were studied by IR, UV, NMR spectroscopic methods and quantum chemistry. When UV irradiated, tricarbonyl complexes lose a CO molecule to form dicarbonyl chelates stabilized by intramolecular coordination of the manganese atom to the ring substituent, the color of the solution being changed. In the closed system, the CO molecule released attaches to the intermediate again, and the initial color recovers. The process can be multiply repeated. In the case of cymantrenes with bifunctional substituents, photochromic systems were discovered where the color change occurs due to linkage isomerization of the manganese atom with a substituent in the dicarbonyl chelates. The spectral data agree well with the results of DFT quantum chemical calculations. The work was supported by Russian Academy of Sciences grant CMS-1.